What is semiquantum mechanics?

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Abstract

Semiclassical approximations to quantum dynamics are almost as old as quantum mechanics itself. In the approach pioneered by Wigner, the evolution of his quasiprobability density function on phase space is expressed as an asymptotic series in increasing powers of Planck's constant, with the classical Liouvillean evolution as leading term. Successive semiclassical approximations to quantum dynamics are defined by successive terms in the series. We consider a complementary approach, which explores the quantum-clssical interface from the other direction. Classical dynamics is formulated in Hilbert space, with the Groenewold quasidensity operator as the image of the Liouville density on phase space. The evolution of the Groenewold operator is then expressed as an asymptotic series in increasing powers of Planck's constant. Successive semiquantum approximations to classical dynamics are defined by successive terms in this series, with the familiar quantum evolution as leading term.

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1 Introduction

Wigner introduced his famous quasiprobability density function on phase space in order to consider semiclassical approximations to the quantum evolution of the density matrix [1]. For a system with one degree of freedom and classical Hamiltonian

$$H = p^2/2m + V(q)\,, \tag{1}$$

he found for the evolution of the Wigner function $W(q,\, p,\, t)$,

$$\begin{aligned} W(q,\, p,\, t)_t = V'(q)\, W(q,\, p,\, t)_p - \frac{p}{m}\, W(q,\, p,\, t)_q \\ -\frac{\hbar^2}{24}\left\{ V'''(q) W(q,\, p,\, t)_{ppp} - \frac{3p}{m}\, V''(q) W(q,\, p,\, t)_{qpp} \right. \\ \left. + \frac{3}{m}\, V'(q) W(q,\, p,\, t)_{qqp} \right\} + \mathrm{O}(\hbar^4)\,. \end{aligned} \tag{2}$$

Here we have introduced the notation $V'(q)$ for $dV(q)/dq$ and W_p for $\partial W/\partial p$, *etc.* The first two terms on the RHS in (2) define the classical Liouvillean evolution, while the terms of order $\hbar^2$ define the first semiclassical approximation to the full quantum evolution of the Wigner function, and so on.

Following the subsequent works of Groenewold [2] and Moyal [3], we now recognize the RHS of (2) as the expansion in ascending powers of $\hbar$ of the star, or Moyal, bracket of the Hamiltonian H and the Wigner function W,

$$\{H,\, W\}_\star = \frac{2}{\hbar}\, H\, \sin\left(\hbar J/2\right)\, W\,, \qquad J = \frac{\partial^L}{\partial q}\frac{\partial^R}{\partial p} - \frac{\partial^L}{\partial p}\frac{\partial^R}{\partial q}\,,$$

$$W_t = \{H,\, W\}_\star = H\, J\, W - \frac{\hbar^2}{24}\, H\, J^3\, W + \mathrm{O}(\hbar^4)\,. \tag{3}$$

Here the superscripts R and L in the Janus operator J indicate the directions in which the differential operators act. The leading term $H\,J\,W$ in the last equation represents the Poisson bracket of H and W, and corresponds to the first two terms on the RHS in (2).

All this is very well known. It is a central ingredient of the so-called phase space formulation of quantum mechanics [4, 5], where operators on Hilbert space are mapped into functions on phase space, and in particular the density operator is mapped into the Wigner function.

Less well known is that, in a completely analogous way, classical mechanics can be reformulated in Hilbert space [2, 6, 7], with the classical Liouville density mapped into a quasidensity operator [8–10] that we have called elsewhere [11] the Groenewold operator. The evolution of this operator in time is defined by what we have called [7] the odot bracket, and

the expansion of this bracket in ascending powers of $\hbar$ defines a series of semiquantum approximations to classical dynamics, starting with the quantum commutator.

In this way, we explore the classical-quantum interface in a new way, approaching classical mechanics from quantum mechanics, which is now regarded as a first approximation. So we stand on its head the traditional approach, which approaches quantum mechanics from classical mechanics, regarded as a first approximation.

2 The Weyl-Wigner transform

In order to see how this works, we recall firstly [4, 5, 12] that the phase space formulation of quantum mechanics is defined by the Weyl-Wigner transform $\mathcal{W}$, which maps operators $\hat{A}$ on Hilbert space into functions A on phase space,

$$A = \mathcal{W}(\hat{A})\,, \qquad A = A(q,\,p)\,, \tag{4}$$

and in particular defines the Wigner function $W = \mathcal{W}(\hat{\rho}/2\pi\hbar)$, where $\hat{\rho}$ is the density matrix defining the state of the quantum system. Then

$$\langle\hat{A}\rangle(t) = \mathrm{Tr}(\hat{\rho}(t)\hat{A}) = \int A(q,\,p)\,W(q,\,p,\,t)\,dq\,dp = \langle A\rangle(t)\,,$$
$$\int W(q,\,p,\,t)\,dq\,dp = 1\,, \tag{5}$$

but W is not in general everywhere nonnegative; it is a quasiprobability density function.

In more detail, A is defined by first regarding $\hat{A}$ as an integral operator with kernel $A_K(x,\,y) = \langle x|\hat{A}|y\rangle$ in the coordinate representation, and then setting

$$A(q,\,p) = \mathcal{W}(\hat{A})(q,\,p) = \int A_K(q - x/2,\, q + x/2)\, e^{ipx/\hbar}\,dx\,. \tag{6}$$

The transform of the operator product on Hilbert space then defines the noncommutative star product on phase space,

$$\mathcal{W}(\hat{A}\hat{B}) = A \star B\,, \tag{7}$$

leading to the star bracket as the image of $(1/i\hbar\times)$ the commutator,

$$\mathcal{W}([\hat{A},\,\hat{B}]/i\hbar) = (A\star B - B\star A)/i\hbar = \{A,\,B\}_\star\,. \tag{8}$$

It can now be seen that the quantum evolution of the density matrix

$$\hat{\rho}_t = \frac{1}{i\hbar}[\hat{H},\,\hat{\rho}]\,, \tag{9}$$

is mapped by the Weyl-Wigner transform $\mathcal{W}$ into the evolution equation for the Wigner function

$$W_t = \{H, W\}_\star \tag{10}$$

as in (3), so leading to the sequence of semiclassical approximations as described in the Introduction. In (9), $\hat{H}$ is the quantum Hamiltonian operator, so that $H = \mathcal{W}(\hat{H})$.

In order to define semiquantum approximations to classical dynamics, we begin by considering the inverse Weyl-Wigner transform $\mathcal{W}^{-1}$, which maps functions A on phase space into operators $\hat{A}$ on Hilbert space, so enabling a Hilbert space formulation of classical mechanics [6,7]. We have

$$A_K(x,y) = \mathcal{W}^{-1}(A)_K(x,y) = \frac{1}{2\pi\hbar}\int A([x+y]/2,\, p)\, e^{ip(x-y)/\hbar}\, dp\,, \tag{11}$$

which defines the kernel of $\hat{A}$, and hence $\hat{A}$ itself, in terms of A. In particular the Groenewold operator $\hat{G}(t)$ is defined as $\hat{G} = \mathcal{W}^{-1}(2\pi\hbar\rho)$. Then

$$\langle A\rangle(t) = \int A(q,\, p)\, dq\, dp = \mathrm{Tr}(\hat{A}\hat{G}(t)) = \langle\hat{A}\rangle\,,$$

$$\mathrm{Tr}(\hat{G}(t)) = 1\,, \tag{12}$$

but $\hat{G}$ is not nonnegative definite in general; it is a quasidensity operator.

It can be seen that the development so far is completely analogous to the development of the phase space formulation of quantum mechanics. We can use $\mathcal{W}^{-1}$ to map all of classical mechanics into a Hilbert space formulation [6,7]. To complete the story, we need to say what happens to the classical evolution of the Liouville density

$$\rho_t = H\, J\, \rho \tag{13}$$

under the action of $\mathcal{W}^{-1}$. Obviously the LHS maps into $\hat{G}_t$; the question is, what happens to the Poisson bracket on the RHS.

3 The odot product and odot bracket

To proceed, we note firstly by analogy with the definition of the star product that we can define a commutative odot product of operators on Hilbert space

$$\hat{A}\odot\hat{B} = \mathcal{W}^{-1}(AB)\,. \tag{14}$$

This is an interesting product, quite distinct from the well known Jordan product of operators, which is also commutative. Unlike the Jordan

product, however, this odot product is associative. Some of its other characteristic properties have been described elsewhere [6, 7, 13].

Next we note that $A_q = \{A,\, p\}_\star$ so that

$$\mathcal{W}^{-1}(A_q) = \frac{1}{i\hbar}[\hat{p},\, \hat{A}] = \hat{A}_q\,, \quad \text{say,} \tag{15}$$

where $\hat{p} = \mathcal{W}^{-1}(p)$. Similarly, we define

$$\mathcal{W}^{-1}(A_p) = \frac{1}{i\hbar}[\hat{A},\, \hat{q}] = \hat{A}_p\,,$$

$$\mathcal{W}^{-1}(A_{qp}) = \frac{1}{(i\hbar)^2}[[\hat{p},\, \hat{A}],\, \hat{q}] = \hat{A}_{qp}\,, \quad \textit{etc.} \tag{16}$$

Then

$$\mathcal{W}^{-1}\,(A\,J\,B) = \hat{A}_q \odot \hat{B}_p - \hat{A}_p \odot \hat{B}_q = \frac{1}{i\hbar}[\hat{A},\, \hat{B}]_\odot\,, \quad \text{say}\,, \tag{17}$$

which defines the odot bracket as the inverse image of $i\hbar\times$ the Poisson bracket. From the Poisson bracket it inherits antisymmetry and a Jacobi identity.

Our next task is to find an expansion of the odot bracket in ascending powers of $\hbar$, analogous to the expansion (3) of the star bracket, in order to define a sequence of semiquantum approximations to classical dynamics.

4 Semiquantum mechanics

We set

$$M = \frac{2}{\hbar}\sin\left(\frac{\hbar J}{2}\right)\,, \tag{18}$$

so we can write for any two functions A and B,

$$\{A,\, B\}_\star = A\,M\,B\,, \tag{19}$$

and note therefore that

$$\mathcal{W}^{-1}(A\,M\,B) = \frac{1}{i\hbar}[\hat{A},\, \hat{B}]\,. \tag{20}$$

Next we write the Poisson bracket as

$$A\,J\,B = A\,\frac{\hbar J/2}{\sin(\hbar J/2)}\,M\,B \tag{21}$$

and, noting that

$$\frac{\theta}{\sin(\theta)} = 1 + \theta^2/6 + 7\theta^4/360 - \ldots \tag{22}$$

we obtain from (20) and (16) that

$$\mathcal{W}^{-1}(A\,J\,B) =$$

$$\frac{1}{i\hbar}[\hat{A},\,\hat{B}] - \frac{i\hbar}{24}\Big([\hat{A}_{qq},\,\hat{B}_{pp}] - 2[\hat{A}_{qp},\,\hat{B}_{qp}] + [\hat{A}_{pp},\,\hat{B}_{qq}]\Big) + \mathrm{O}(\hbar^3)\,. \tag{23}$$

Now we can answer the question raised at the end of Section 2. Applying $\mathcal{W}^{-1}$ to both sides of (13), we obtain

$$\hat{G}_t =$$

$$\frac{1}{i\hbar}[\hat{H},\,\hat{G}] - \frac{i\hbar}{24}\Big([\hat{H}_{qq},\,\hat{G}_{pp}] - 2[\hat{H}_{qp},\,\hat{G}_{qp}] + [\hat{H}_{pp},\,\hat{G}_{qq}]\Big) + \mathrm{O}(\hbar^3)\,. \tag{24}$$

Thus we see the evolution of $\hat{G}$ in Hilbert space, which is equivalent to the classical evolution of the Liouville density ρ in phase space, is given as a series in ascending powers of $\hbar$. Keeping successively more terms in the series, we define a sequence of approximations to the classical evolution. Note that the lowest order term is just the quantum evolution, which now appears as the lowest order approximation to classical dynamics. As we add more and more terms, we have the possibility to explore the classical-quantum interface starting from the quantum side. This is completely complementary to what we normally do with semiclassical approximations to quantum mechanics.

5 Examples

J.G. Wood and I have explored semiquantum and semiclassical approximations for simple nonlinear systems with one degree of freedom [14]. Rather than Hamiltonians of the form (1), we considered

$$H \;=\; E\sum_{k=0}^{K} b_k\,(H_0/E)^k\;, \tag{25}$$

where H_0 is the simple harmonic oscillator Hamiltonian

$$H_0 \;=\; p^2/2m + m\omega^2q^2/2\,, \tag{26}$$

and E, b_k are constants. These have the advantage that they are analytically tractable, but still show characteristic differences between the classical and quantum evolutions [15]. In particular we considered

$$H_2 = H_0^2/E\,, \qquad \hat{H}_2 = \mu\hbar\omega\,(\hat{N}^2 + \hat{N} + 1/4)\,,$$

$$H_3 = H_0^3/E^2\,, \quad \hat{H}_3 = \mu^2\hbar\omega\,(\hat{N}^3 + 3\hat{N}^2/2 + 2\hat{N} + 3/4)\,,$$

$$\text{where}\quad \hat{H}_0 = \hbar\omega\,(\hat{N} + 1/2)\,, \qquad \mu = \hbar\omega/E\,, \tag{27}$$

with $\hat{H} = \mathcal{W}^{-1}(H)$ in each case, and $\hat{N}$ the usual oscillator number operator.

As an initial Liouville density on phase space, we took a Gaussian ρ for which the initial Groenewold operator $\hat{G} = \mathcal{W}^{-1}(2\pi\hbar\rho)$ equals a true density operator, namely the density operator for a pure coherent state. Differences between the classical and quantum evolutions of such an initial state, with the Hamiltonians H_2 and $\hat{H}_2$, respectively, are immediately apparent in the phase space plots Fig. 1 and Fig. 2. Under the classical evolution, the density stays positive everywhere, but develops "whorls," whereas under the quantum evolution, the density (Wigner function) becomes negative on some regions (shown in white) and is periodic [15]. Conversely, under the classical dynamics, the Groenewold operator $\hat{G}$ develops negative eigenvalues [8–11, 16], whereas under the quantum evolution, such an initial pure-state density operator stays positive definite, with eigenvalues 0 and 1. Simliar remarks apply with the Hamiltonians H_3 and $\hat{H}_3$.

There is no nontrivial semiquantum or semiclassical approximation "in between" the classical and quantum dynamics for the Hamiltonians H_2 and $\hat{H}_2$. Each of the series (3) and (24) has just two terms in this case. For the series (3), the leading term defines the classical evolution, and adding the next term produces the full quantum dynamics. Similarly, for the series (24), the leading term defines the quantum evolution, and adding the next term produces the full classical dynamics.

To see interesting differences betweem semiclassical and semiquantum approximations, we considered H_3 and $\hat{H}_3$, for which there are three terms in each of the series (3) and (24). Thus we can compare the classical evolution and the first semiclassical approximation to quantum dynamics, and also the quantum evolution and the first semiquantum approximation to classical dynamics. In Fig. 3 we plot the expectation values of q, p in the classical and semiclassical cases, calculated at each time using the Liouville density ρ or the Wigner function W as in (5), and also the expectation values of $\hat{q}$ and $\hat{p}$ in the quantum and semiquantum cases, calculated at each time using the density operator $\hat{\rho}$ or the Groenewold operator $\hat{G}$ as in (12). From our results it is already clear that semiquantum and semiclassical approximations provide different information about the interface between classical and quantum behaviours.

These expectation values compare "classical-like" properties of the different evolutions. We also considered "quantum-like" properties of the diferent evolutions, in particular the largest and smallest eigenvalues of $\mathcal{W}^{-1}(\rho)$ and $\mathcal{W}^{-1}(W)$ in the classical and semiclassical cases, and the largest and smallest eigenvalues of $\hat{\rho}$ and $\hat{G}$ in the quantum and semiquantum cases. The results are shown in Fig. 4.

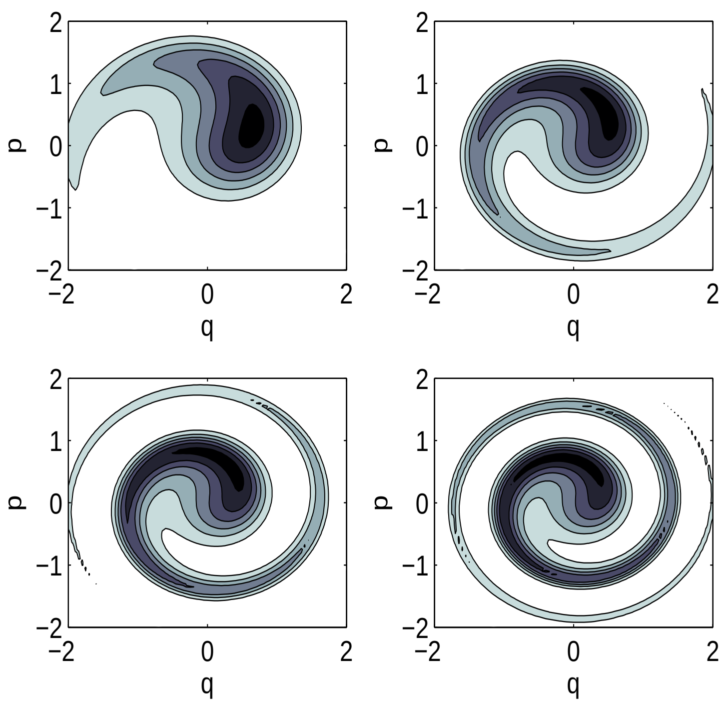

Figure 1: Density plots showing the classical evolution of an initial Gaussian density centered at $q_0 = 0.5$, $p_0 = 0$ as generated by the Hamiltonian $H = H_0^2/E$. The parameters m, ω, E have been set equal to 1, and the times of the plots are, from left to right and top to bottom, $t = \pi/4$, $t = \pi/2$, $t = 3\pi/4$ and $t = \pi$.

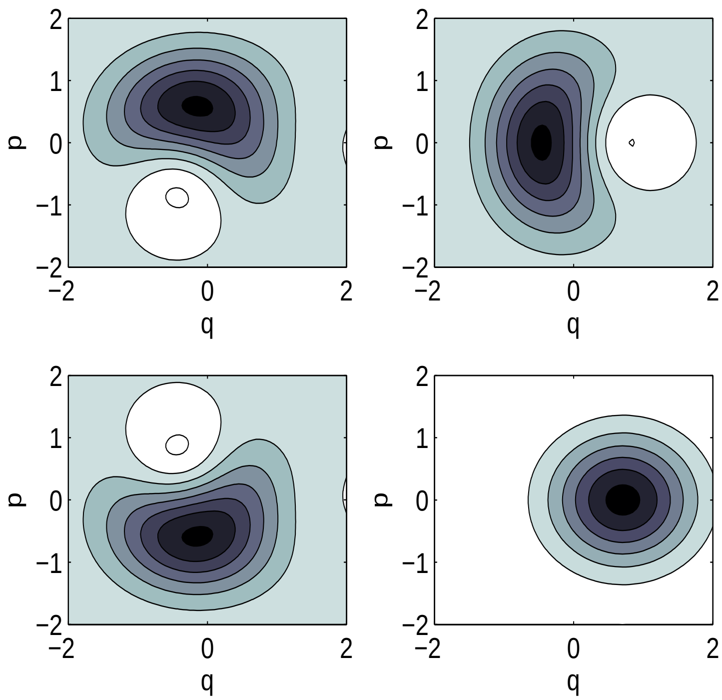

Figure 2: Quantum evolution of an initial Gaussian Wigner function, with the same parameter values used in Figure 1, and shown at the same times. Regions on which the pseudo-density becomes negative are shown in white in the first three plots.

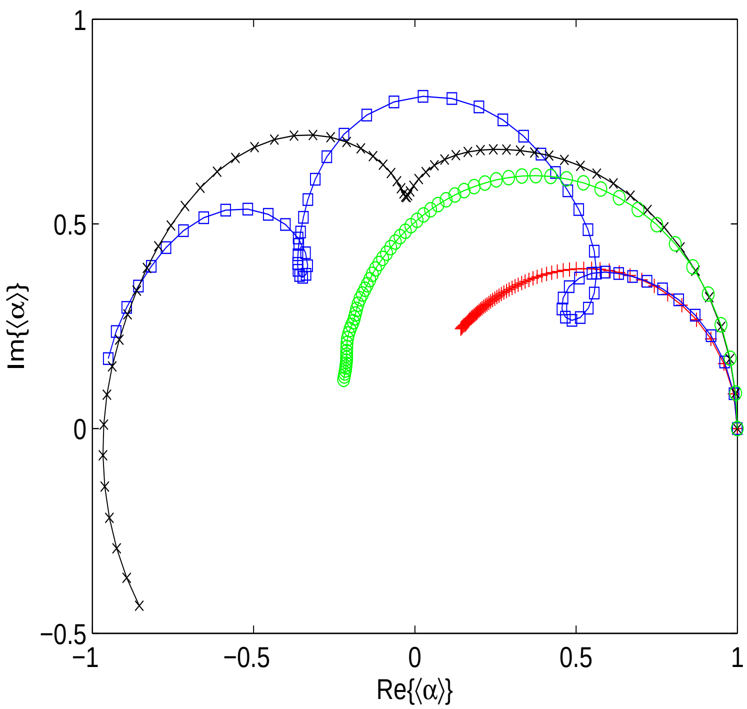

Figure 3: Comparison of first moments of $\alpha = (q + ip)/\sqrt{2}$ for classical, semiquantum, quantum and semiclassical evolutions generated by the Hamiltonian $H = H_0^3/E^2$. Points on the classical, quantum, semiclassical and semiquantum curves are labelled by $+$, x, o and $\Box$, respectively. The evolution is over the time-interval $[0, \pi]$ and again $m = \omega = E = 1$, with $\mu = 1/2$, $\alpha_0 = 0.5$.

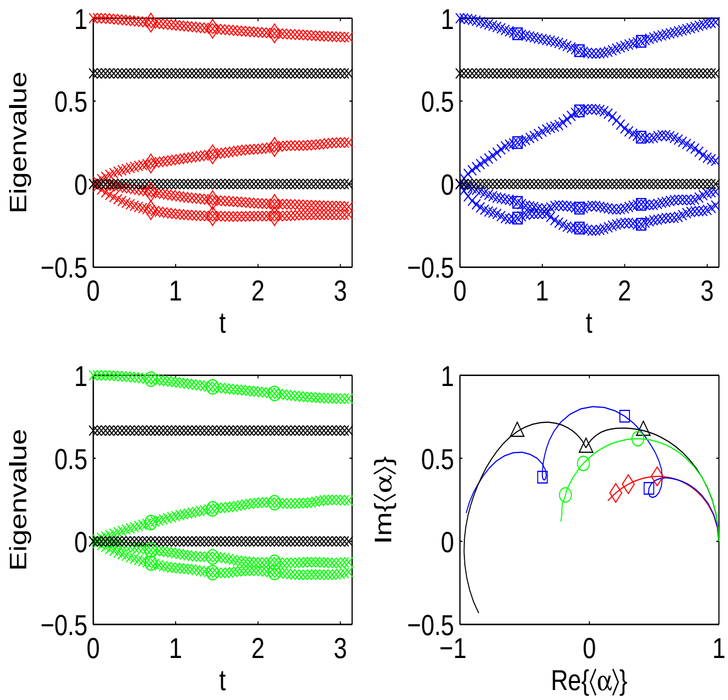

Figure 4: Comparison of largest two and least two eigenvalues for, from left to right and top to bottom, classical, semiquantum and semiclassical evolutions generated by $H = H_0^3/E^2$, for the time interval $[0, \pi]$, and with $m = \omega = E = 1$ and $\mu = 1/2$, $\alpha_0 = 0.5$. The evolution of the first moment is reproduced from Fig. 3 in the graph at bottom right for comparison. Each of the other graphs also features the quantum spectrum $\{0, 1\}$ and in all graphs the values at the time-points $t = 1, 2, 3$ are marked $\Diamond$ (classical), o (semiclassical), $\triangle$ (quantum) and $\Box$ (semiquantum).

6 Conclusions

Semiquantum mechanics opens a new window on the interface between classical and quantum mechanics. Our investigations of examples as described above have not yet gone very far, but already we can say that semiquantum approximations show characteristic differences from semiclassical approximations for a given nonlinear system. More details are given in Ref. [14].

It is important to explore the nature of semiquantum approximations for other systems. For example, from the classical Hamiltonian H as in (1), we obtain

$$\hat{H} = \hat{p}^2/2m + V(\hat{q})\,, \tag{28}$$

and substituting in (24), we get for the evolution of the Groenewold operator in such cases

$$\hat{G}_t = \frac{1}{i\hbar}[\hat{p}^2/2m + V(\hat{q}),\, \hat{G}] - \frac{i\hbar}{24}[V''(\hat{q}),\, \hat{G}_{pp}] + \mathrm{O}(\hbar^3)\,, \tag{29}$$

which is to be compared with Wigner's famous formula (2) for the evolution of the Wigner function. The implications of (29) for various important choices of V, in particular exactly solvable cases, should be examined.

Of even more interest of course are systems with more degrees of freedom that show chaos at the classical level. For such systems it should be particularly interesting to consider differences in the spectral properties of $\hat{G}$ at different times in different approximations, in classically chaotic or integrable regimes, as well as the different behaviours of expectation values of important phase space variables.

We hope to investigate some of these problems.

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